

Analytical approximations of the Lindhard equations describing radiation effects

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Abstract

Starting from the general Lindhard theory describing the partition of particles energy in materials between ionisation and displacements, analytical approximate solutions have been derived, for media containing one and more atomic species, for particles identical and different to the medium ones. Particular cases, and the limits of these equations at very high energies are discussed.

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1 Introduction

The characteristics of semiconductor devices and other crystalline materials used in high fluences of particles are strongly affected by the effects of radiation. In the recent years, important results have been achieved in the radiation damage analysis, but not all the degradation mechanisms have been completely understood up to now. After the interaction of the radiation field with the semiconductor material, mainly two classes of degradation effects were observed: surface damage and bulk material damage, due to the displacement of atoms from their sites in the lattice.

If heavy particles as pions, protons, neutrons, ions, etc., produce both surface and bulk damages, for electrons and gammas the effects are dominantly produced at the surface. The surface effects are not a main obstacle to semiconductor device operation, while the bulk ones have a much greater importance. The disruption of the symmetry of the crystal, consequence of the bulk effects, causes the formation of energy levels in the normally forbidden region between the valence and conduction bands, altering the material properties.

The process of partitioning the energy of the recoil nuclei (produced due the interaction of the incident particle with the lattice site nucleus) in new interactions processes, between electrons (ionisation) and atomic motion (displacements) is considered in the general form, in the frame of the Lindhard theory [1] .

Up to now, there exist in the literature some calculations of the Lindhard curves for some crystalline materials: diamond [2,3], Si [4,5], GaAs [6], InP [7], and GaP, InAs, InSb [8], in Al and some scintillator materials [9].

The knowledge of the Lindhard energy partitioning curves is essential, together with the detailed nuclear interaction mechanisms, in the correct evaluation of the concentration of primary defects produced in materials that work in intense fields of radiation. In this paper, we present the concrete equations necessary in the analytical calculations of these curves.

2 General hypothesis and analytical approximations of Lindhard equations

The general process considered in the study of the interaction between the incident particle and the solid is the following: the particle, heavier than the electron, with electrical charge or not, interacts with the electrons and with the nuclei of the semiconductor lattice. It loses its energy in several processes, which depend on the nature of the particle and on its energy. The effect of the interaction of the incident particle with the electrons of the target is the ionisation. The quantity characteristic for this process is the energy loss dE/dx (stopping power). The nuclear interaction between the incident particle and the lattice nuclei produces bulk defects. As a result of the interaction, depending on the energy and on the nature of the incident particle, one or more light particles are formed, and usually one (or more) heavy recoil nuclei. The nucleus has charge and mass numbers lower or equal with that of the medium. After this interaction process, the recoil nucleus or nuclei are displaced from the lattice positions in interstitials. Then, the primary knock-on nucleus, if its energy is large enough, can produce the displacement of a new nucleus, and the process continues as long as the energy of the colliding nucleus is

higher than the threshold for atomic displacements. This phenomenon can be regarded as a cascade process. We denote by primary displacements all the displacements produced as a result of primary interactions, without any further rearrangement of the vacancies and interstitials. The physical quantity characterising the process is the concentration of primary defects (or related quantities, for example the non ionising energy loss) produced per unit of fluence of the incident particles.

In all the subsequent discussions, the primary recoil will be the particle whose energy partition is to be calculated. As specified before, the primary recoil is either a nucleus of the medium, or a nucleus with a lower mass and charge numbers. As a consequence, for each medium a whole family of curves can be obtained. Also these Lindhard curves can be directly used in the evaluation of the damage produced in materials by ion beams, if the energy of particles in the beam is identified with recoils energy.

The incident particle has an initial energy E , and, due to the interaction with the target during the slowing down, this energy is transferred, on the one side to atoms (the quantity E_1), and on the other side to electrons (the quantity E_2). Obviously:

$$E = E_1 + E_2 \quad (1)$$

In accord with [1], the equation satisfied by E_1 , as a function of the energy E , is:

$$\int d\sigma_{n,e} \left[E_1 \left(E - T_n - \sum_i T_{ei} \right) - E_1(E) + E_1(T_n - U) + \sum_i E_{1e}(T_{ei} - U_i) \right] = 0 \quad (2)$$

where $d\sigma_{n,e}$ are the differential cross sections corresponding to particle scattering on nucleus and electrons, $T_n(T_{ei})$ represent the energies transferred to nucleus (and respectively to electrons), U is the energy wasted in disrupting the atomic binding, and U_i are the corresponding ionisation energies, with summation over all electrons.

The equation takes into consideration all the steps of the interaction until the transferred energy is lower than the threshold energy for displacements. In this general form, the equation is practically impossible to be solved. It has been simplified [1], using some physical approximations: the electrons do not produce recoil nuclei with appreciable energy, so that the function E_{1e} (for electrons), can be obtained separately; the binding energy of the atom in the lattice can be neglected; the energy transferred to electrons and respectively

to nuclei is small in respect to the particle energy, and electronic and nuclear collisions can be separated. More, the energy transferred from electrons to nuclei is negligible, $E_{1e} = 0$.

Using the up - mentioned approximations, the equation for the function E_1 becomes:

$$(S_n + S_e) E_1' = \int_{T=0}^E E_1(T) \frac{d\sigma_n}{dT} dT \quad (3)$$

where $S_{n,e} = \int T_{n,e} d\sigma_{n,e}$ represent the stopping cross sections for nuclei and electrons. The boundary condition for the equation 3 is: $E_1(E)/E \rightarrow 1$ for $E \rightarrow 0$.

The parameter $\xi(E)$, defined as:

$$\xi(E) = \frac{S_e}{S_n} \quad (4)$$

represents a measure of the division of energy dissipation into electronic and atomic motions. For the simplest case, of a medium consisting of only one atomic species, and of the particle - primary recoil identical to the particles of the medium ($Z_{part} = Z_{med} = Z$, and $A_{part} = A_{med} = A$), and for an electronic cross section $S_e \propto E^{1/2}$ and with S_n derived from a Thomas-Fermi potential, it was shown [1] that for $\xi(E)$ there exist roughly three distinct energy regions. In the first one, the nuclear stopping is dominating, and relatively little energy goes into electronic motion; in the second region, the nuclear stopping start decreasing, while the electronic one increases as $E^{1/2}$, so the quantity $\xi(E)$ increases rapidly, and the fraction of the energy that goes into electronic motion increases correspondingly; in the third region, the electronic stopping starts decreasing, while $\xi(E)$, though still increasing, approaches an asymptotic value.

It is convenient to look for analytical approximate solutions. The simplest case to treat mathematically is that of a power low potential, $V(r) \propto r^{-s}$, corresponding to nuclear scattering. In this case, the equation 2 can be replaced with a differential equation whose solution is the hypergeometric function. In the first region an potential represents a good approximation. The solution is:

$$E_1(E) \propto E_c \left\{ -12 + 6 \left[1 + 2(E_c/E)^{1/2} \right] \cdot \log \left(1 + (E_c/E)^{1/2} \right) \right\} \quad (5)$$

where $E_c \propto Z \cdot A$ is the upper limit of the first energy region. In the limit $E/E_c \ll 1$, the solution for $E_1(E)$ can be expressed even simpler, as a power

series in $(E/E_c)^{1/2}$. The solution described by equation 5 is a fast increasing one on energy.

In the second region, the cross section could be modelled using the Rutherford scattering formula, i.e. using $s = 4/3$. The analytical formula derived for E_1 [1] is:

$$E_1(E) \propto C_1 E_b \left\{ 1 - \frac{1}{4\sqrt{2}} \xi^{-1/4} \log \frac{\xi^{1/2} + \sqrt{2}\xi^{1/4} + 1}{\xi^{1/2} - \sqrt{2}\xi^{1/4} + 1} - \frac{1}{2\sqrt{2}} \xi^{-1/4} \arctan \frac{\sqrt{2}\xi^{1/4}}{1 - \xi^{1/2}} \right\} + C_2 \xi^{-1/4} E_b^{-1/4} \quad (6)$$

where $\xi(E)$ defined by eq. 4 is given by E/E_b , E_b being the energy at which the two stopping cross sections are equal; E_b has the same dependence on A and Z as E_c , C_1 is of the order of unity, and has the approximate expression:

$$C_1 \simeq \frac{12}{x^2} + 6 \frac{(x+1)(x-2)}{x^2} \cdot \log(x+1) \quad (7)$$

with $x \equiv E_b/E_c$ and C_2 is small, usually negative. The function $E_1(E)$ must be continuous at the boundary of the two regions. In this region, E_1 has a much slower increasing slope on E , approaching the plateau corresponding to the third region, and given by the asymptotic limit.

For particles that do not belong to the medium, but for unielement media, the problem can be solved in principle starting from the solution corresponding to particles identical with the medium ones, obtained from eqs. 5 and 6, and denoted by $\epsilon(E)$. So, the equation whose solution is of interest is:

$$E'_1(E) \cdot S_{e,part} = \int d\sigma_{part} [\epsilon(E-T) - \epsilon(E) + \epsilon(T)] \quad (8)$$

where is the electronic stopping cross section for the ion Z_{part} in the medium Z_{med} , and $d\sigma_{part}$ is the differential cross section for an elastic scattering of the particle on the atom of the medium, with the stopping cross section $S_{n,part}$. In this situation, the division of the energy interval into three regions does not hold more, because, in place of S_e and S_n we have now $S_{e,part}$ and $S_{e,med}$, and $(S_{n,part}, S_{n,med})$ respectively. The case of media containing more than one element is more complicated, and is very difficult to be treated rigorously. A first approximation for the solution of the problem of the energy partition of a particle in a multielement medium is to solve separately for each component, and to use the average weight Bragg additivity. This method has been used in the case of some binary semiconductors [7,8].

3 Particular cases and discussion

In the case of a medium consisting of only one atomic species, but for particles different from the medium, the eqs. 5 and 6 could be still used, as a first approximation, instead of eq. 7, redefining the quantities E_c and E_b . An important distinction is to be made between particles lighter then the medium, and heavier than the medium. While E_b has the same dependence on the characteristics of the particle and medium in both cases:

$$E_b \simeq 5.2 \cdot 10^{-4} \frac{(Z_{part}^{2/3} + Z_{med}^{2/3})^2}{Z_{part}^{1/3}} \frac{A_{part}^3}{(A_{part} + A_{med})^2} \quad (9)$$

(in MeV) E_c has different forms.

For $Z_{part} < Z_{med}$ and $A_{part} < A_{med}$:

$$E_c \simeq 5 \cdot 10^{-4} \frac{(Z_{part}^{2/3} + Z_{med}^{2/3})^2}{Z_{part}^{1/3}} \frac{A_{part}^3}{(A_{part} + A_{med})^2} \quad (10)$$

while for $Z_{part} > Z_{med}$ and $A_{part} > A_{med}$:

$$E_c \simeq 1.25 \cdot 10^{-4} Z_{med} \frac{(A_{part} + A_{med})^2}{A_{part}} \quad (11)$$

For a given medium, consisting of only one atomic species, the family of curves characterising the dependence of the energy channelled into displacements, as a function of the recoils energy, and having the mass and charge numbers ($A_{part} \leq A_{med}$ and $Z_{part} \leq Z_{med}$) as parameters, has the following characteristics:

- The maximum energy transferred into displacements corresponds to particles identical to the medium ones.
- All curves start, at low energies, from the same curve; they have at low energies identical values of the energy spent in displacements, independent on the charge and mass number of the recoil, and, roughly, an dependence.
- At higher energies, the curves start to detach from this main branch. This happens at lower energies if their charge and mass numbers are smaller. Then, the curves present a smooth increase with the energy. This means that at high enough energy of the incident particle, the increase of its energy determines, mainly, an increase of the ionisation loss. The asymptotic limit (E_p) of the

Fig. 1. The displacement energy versus the particle (recoil) energy for C in diamond (continuous line), Si in silicon (dotted line), and respectively Ge in germanium (dashed- dotted line). The asymptotic limits of the displacement energies are also represented. The characteristic energies for the curves are indicated with arrows.

equation 6 depends on the characteristics of the particle and of the medium as:

$$\frac{\left(Z_{part}^{2/3} + Z_{med}^{2/3}\right)^2}{Z_{part}^{1/3}} \frac{A_{part}^3}{(A_{part} + A_{med})^2} \quad (12)$$

In the particular case of a particle belonging to the medium, the value of this energy is proportional to the product of the mass and charge numbers; if, more, $Z \simeq A/2$, as is the case of C in diamond, Si in silicon and Ge in germanium, an $A^{\simeq 2}$ dependence is obtained for E_p .

In Figure 1, the Lindhard curves for C in diamond, Si in silicon and Ge in germanium are presented. The values of corresponding to the boundary between the first and the second energy regions for all three curves are indicated by arrows. The asymptotic limits are also shown at the highest limit of the abscissa. In fact, the solution given by equation 6 is the most important in the evaluation of the bulk damage produced in materials, in accelerator applications. For example, the standard physics programme at LHC is based on an integrated luminosity of $5 \cdot 10^5 \text{ pb}^{-1}$, which corresponds to year of operation, for an annual operation time of $1.9 \cdot 10^7 \text{ s}$. The charged hadrons are produced by the primary interaction proton-proton at 7 GeV, while neutrons are albedo particles. The irradiation background is continuous. The charged hadrons spectra (π^\pm , K^\pm , p , \bar{p}) simulated for various positions inside the tracking cavity of the

Fig. 2. The displacement energy versus particle (recoil) energy for two sets of elements near one another in the periodic table, that form two binary compounds. The first one indicates the particle, the second one the medium. The asymptotic limits (plateau) of the displacement energies are also represented.

CMS [10] suggest that all hadrons have their kinetic energies between 10^{-2} - 20 GeV. Corresponding to these kinetic energies, if only elastic interactions with the detector medium (diamond, silicon, germanium) are considered, the recoil nuclei have energies higher than some MeV, values in the saturation region of the Lindhard curves. The case of binary media has been treated, in a first approximation, as specified before, considering separately the two components, and then weighting with their number in the molecule. If the two components are adjoining each other in the periodic table, as is the case of, e.g., GaAs and InSb, then there is no significant difference in the Lindhard partition energy curves, for element placed between the two elements of the compound. In Figure 2, the Lindhard curves for As in Ga, Ga in As, Sb in In and In in Sb are given. For all of them, the asymptotic limit is also indicated. The curves for Ga and As could be compared with the one corresponding to Ge in germanium, presented in Figure 1. If the two components are far each other in the periodic table, then there are, in principle, two families of curves, one corresponding to the heaviest element, the other to the lightest one, separated by a gap. As an illustration, in Figure 3 the results for P in In and In in P, as well as those for Ga in P and P in Ga are presented. These are useful in the evaluation of radiation defects in the semiconductor compounds GaP and InP. The asymptotic limit of the energy used for displacements is also represented.

Fig. 3. The displacement energy versus particle (recoil) energy for two sets of elements far one another in the periodic table, that form two binary compounds. The first one indicates the particle, the second one the medium. The asymptotic limits of the displacement energies are also represented.

4 Summary

Recent development of accelerator machines conduces to the necessity of the study of radiation effects in a multitude of materials, in intense fields of a large variety of particles, in a high range of energy and at different fluences. As essential factor in the evaluation of radiation effects is the knowledge of the energy partition of slowing down particles, between ionisation and displacements in the lattice of the target. The Lindhard theory gives a detailed description of the calculation procedure for particles identical to the medium and for media consisting of one atomic species, and proposes some approximations for other situations. In the present article, we applied approximate methods for the calculation of the Lindhard curves for particles that do not belong to the medium, both for unielement and compound media. As the asymptotic value of these curves is of much interest for practical applications, the dependence of this value on the characteristics of the particle and medium is given.

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